Co-Optimization of
Fuels & Engines

Co-Optima Emissions and Emissions Control for SI/ACI Multimode Combustion

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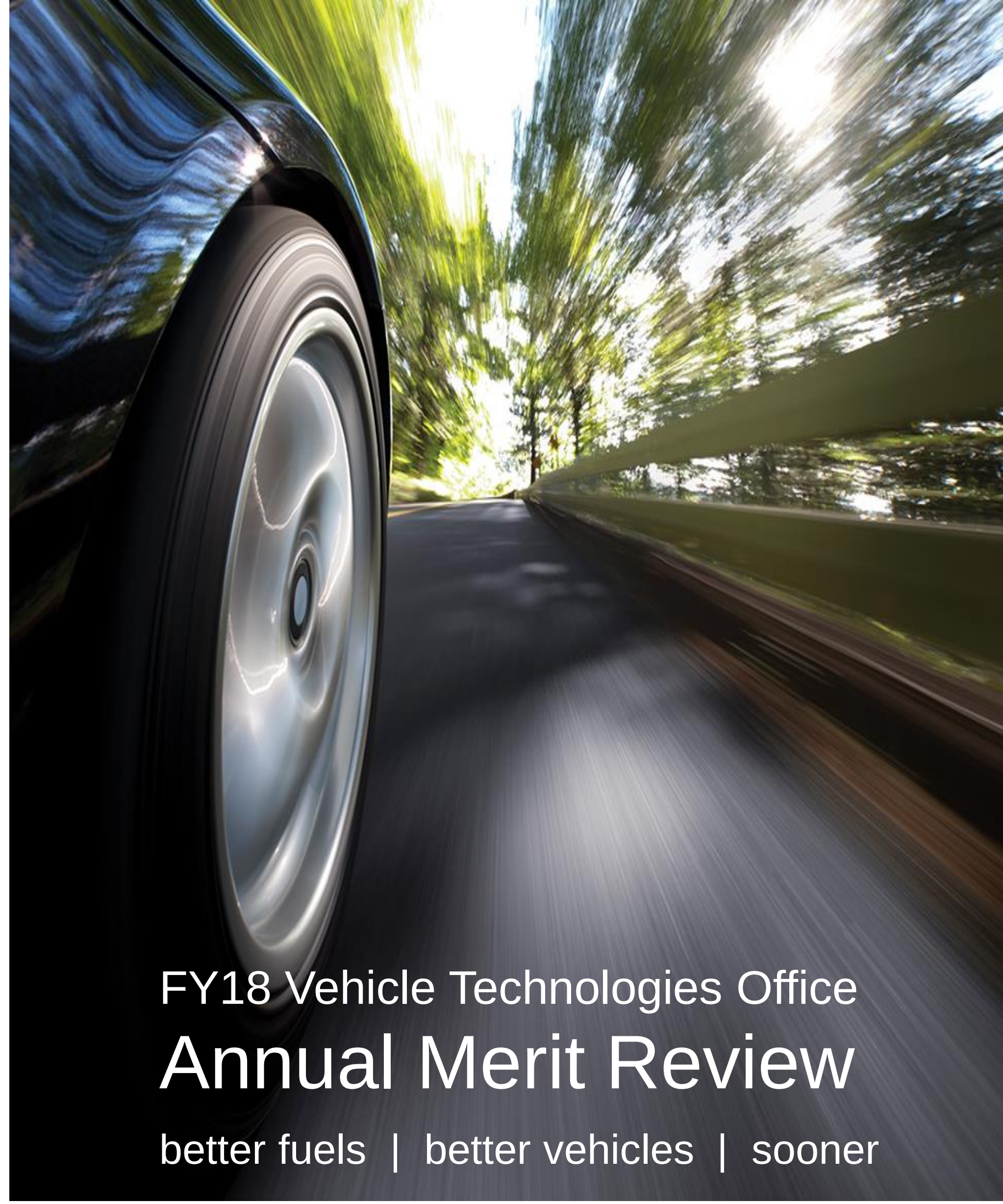
VTO Program Managers: Gurpreet Singh, Kevin Stork, Michael Weismiller

Project # FT073

June 12, 2019



Overview

Timeline

- Project start date: 10/1/2018
- Project end date: 9/30/2021*
- Percent complete: 17%

*Start and end dates refer to three-year life cycle of DOE lab-call projects, Co-Optima is expected to extend past the end of FY19

Budget

	FY18	FY19**
E.1.3.1	$175k	$250k
Co-Optima fuel impacts on SI/ACI emissions control performance MM. ***Pihl (ORNL)***		
E.2.2.5	$350k	$220k
Impact of fuel chemistry on PM emissions across ACI modes within the Multimode operating space. ***DeBusk/ Storey (ORNL)***		

**expected

Barriers from US DRIVE ACEC Roadmap

- U.S. EPA Tier 3 Bin 30 emissions
- Reduced cold start emissions
- "…greater understanding of how new fuels impact advanced combustion strategies and aftertreatment systems"

Collaborations

- Co-Optima partners
  - 9 National Labs, 20+ Universities, 80+ Stakeholder organizations
- Direct communications with OEMs and catalyst suppliers
- CLEERS community (emissions control)
  - OEMS, Universities, and National Labs

Co-Optima Overarching Relevance

Delivering Foundational Science

- The U.S. DOE Co-Optima initiative is delivering foundational science to develop fuel and engine technologies that will work in tandem to achieve efficiency, environmental and economic goals

General Relevance

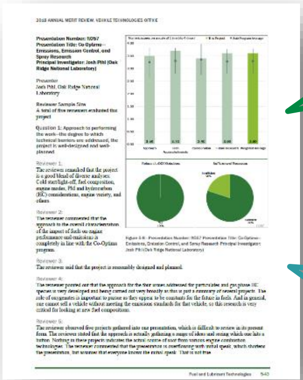
- Internal combustion engines and the use of liquid fuels projected to dominate transportation for many years
- Significant opportunities exist to further improve engine efficiency and corresponding vehicle fuel economy
- Research into better integration of fuels and engines is critical to accelerating progress towards achieving efficiency, environmental and economic goals
- Research addresses engine fuel barriers and opportunities for light-duty boosted SI, medium-duty and heavy-duty MCCI, and ACI combustion approaches

LD = light duty; MD = medium duty; HD = heavy duty; SI = spark ignition;
ACI = advanced compression ignition

Relevance of Emissions Control tasks to overall Co-Optima program

Relevance | Approach | Technical | Collaboration | Future Work

2018 Merit Review



Reviewer 2: "…the approach to the overall characterization of the impact of fuels on engine performance and emissions is completely in line with the Co-Optima program."

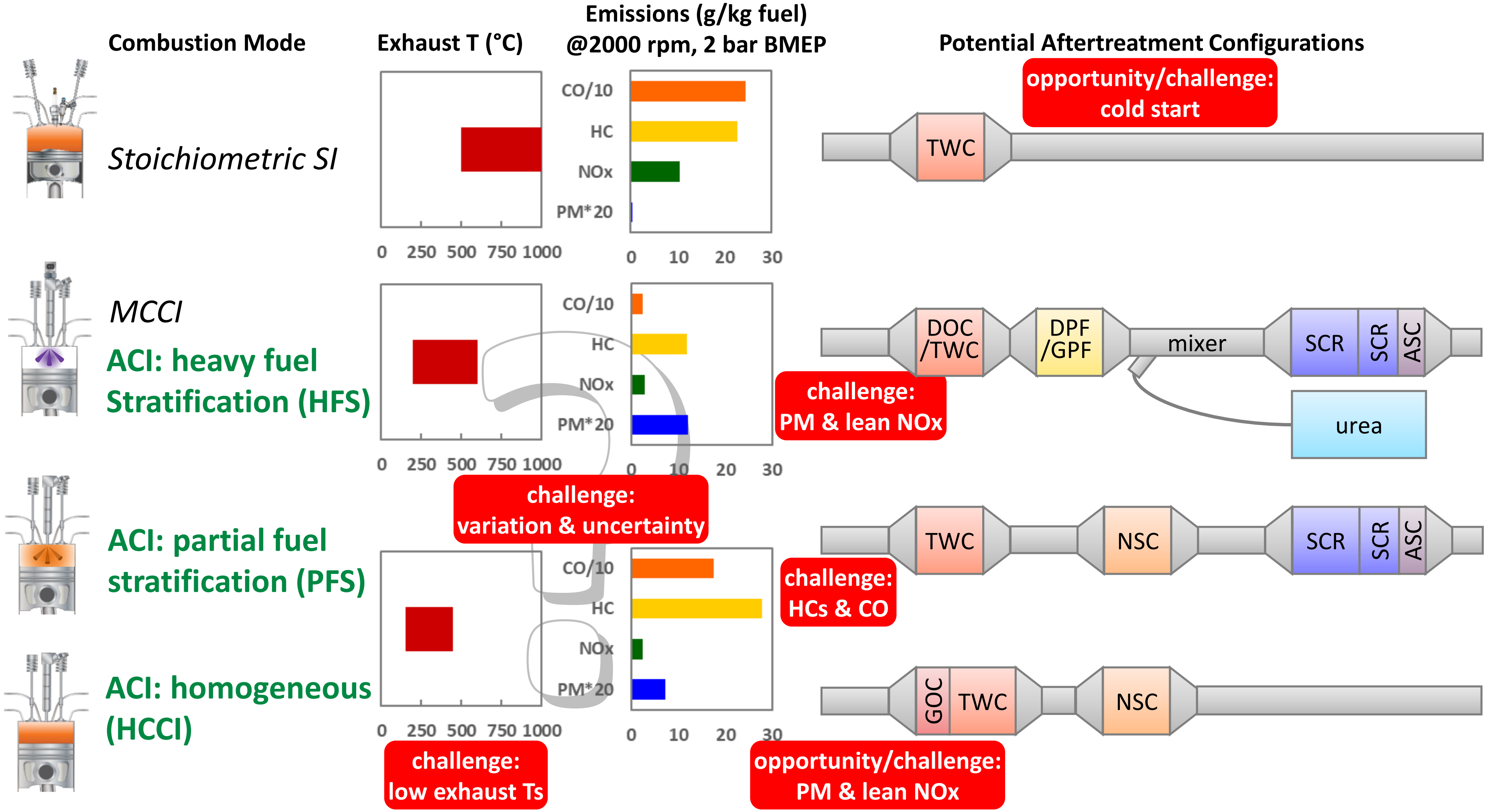
Reviewer 4: "…And in general, one cannot sell a vehicle without meeting the emissions standards for that vehicle, so this research is very critical for looking at new fuel compositions."

- Advanced engines running on high performance fuels <u>must still meet emissions regulations</u>
- Advanced Compression Ignition (ACI) presents a new set of emission challenges that are as yet not completely understood
- Changes in fuel chemistry and combustion strategy impact engine emissions (NOx, CO, PM formation, THC and NMOG speciation)
  - Introducing new challenges & opportunities in emissions and emissions control

We need to understand how fuel chemistry impacts exhaust composition and performance of emission control devices to predict the effects of Co-Optima blendstocks on regulated emissions

Emissions Control Opportunities and Challenges

SI/ACI and ACI engine aftertreatment configurations will be more complex than SI only

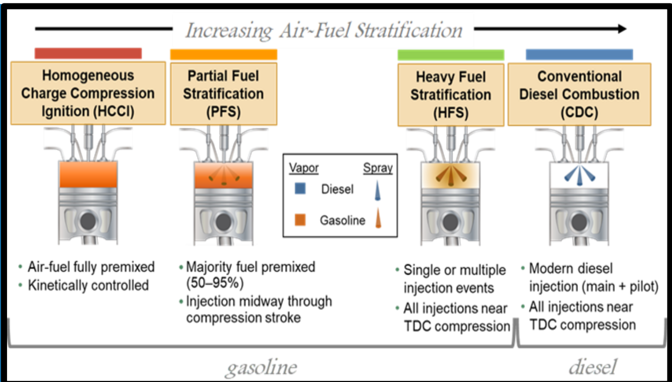


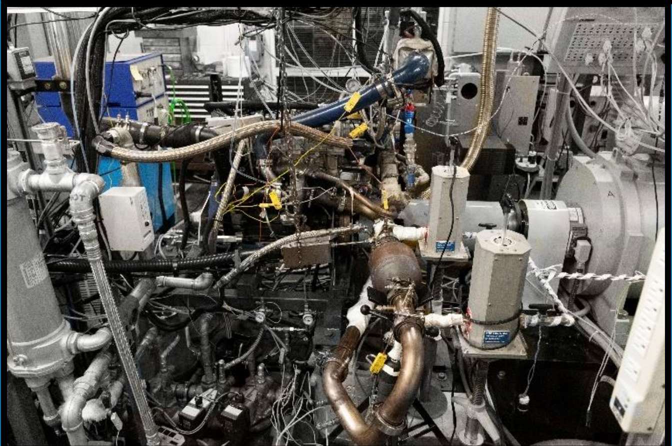
TWC= 3-way catalyst; DOC/GOC = oxidation catalyst; DPF/GPF = particulate filter; SCR = selective catalytic reduction; ASC = ammonia slip catalyst; NSC = NOx slip catalyst

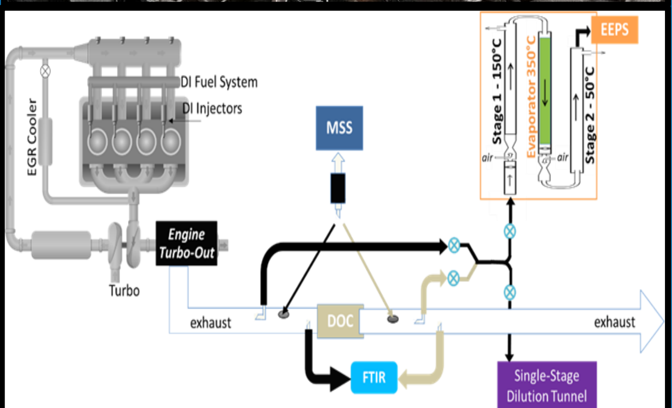
Milestones

Task	Lab	Timing	Description of Milestone or Go/No-Go Decision	Status
E.1.3.1	ORNL	FY18 Q4	Measure TWC light-off temperatures for five fuel blends containing Co-Optima blendstocks to support evaluation of LD merit function term	Complete
E.1.3.5	ORNL	FY18 Q4	Complete PM sampling study on impact of fuels, T, and mixedness conditions on PM from mixed-mode SI/ACI	Complete
E.1.3.1	ORNL	FY19 Q4	Measure TWC light-off of five or more Co-Optima blendstocks under lean conditions to evaluate behavior under ACI operation for SI/ACI multimode engines	On track

E.1.3.5: Fuel Impacts on ACI Particulate Matter (PM) Formation







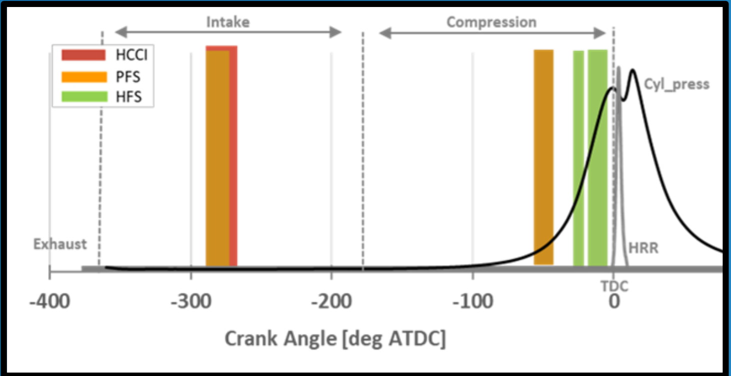
Melanie Moses-DeBusk, John Storey, Sam Lewis, R. Maggie Connatser, and Scott Curran (ORNL)

Relevance:

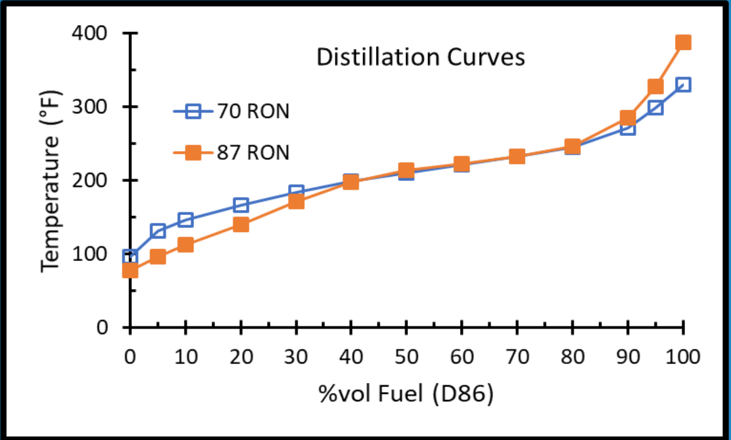
- Advanced engines & fuels must meet emissions standards
- Specific ACI combustion modes and ideal fuel undefined for SI/ACI multimode strategies
  - Air-fuel stratification known to impact emissions in other combustion strategies
  - Engine emission known to be sensitive to fuel properties

Objectives:

- Study impact of air-fuel stratification and fuel properties on ACI emissions
  - Do different stratification levels follow a similar impact trend on PM, HC emissions? Can it be predicted?
  - Do different fuel properties offer emissions trade-offs?



	70 RON	87 RON
Reid Vapor Pressure (RVP, psi)	7.0	11.7
Distillation T50 (F)	210.5	214
Distillation T90 (F)	271.2	285
Aromatics (vol%)	15.5%	19.4%
Olefins (vol%)	0.3%	3.7%
Saturates (vol%)	84.2%	75.7%
MON	68	83



Approach:

Study how bookends of ACI air-fuel stratification impact PM and gaseous emissions and further influence of fuel properties

Multiple ACI modes available for multimode engines

- Major difference in possible modes corresponds to air-fuel stratification
- Studied ACI bookends @ 2000rpm, 4-5bar:
  - Fully mixed/ no stratification: HCCI
  - Mostly mixed/ low stratification: PFS
  - High fuel stratification: HFS

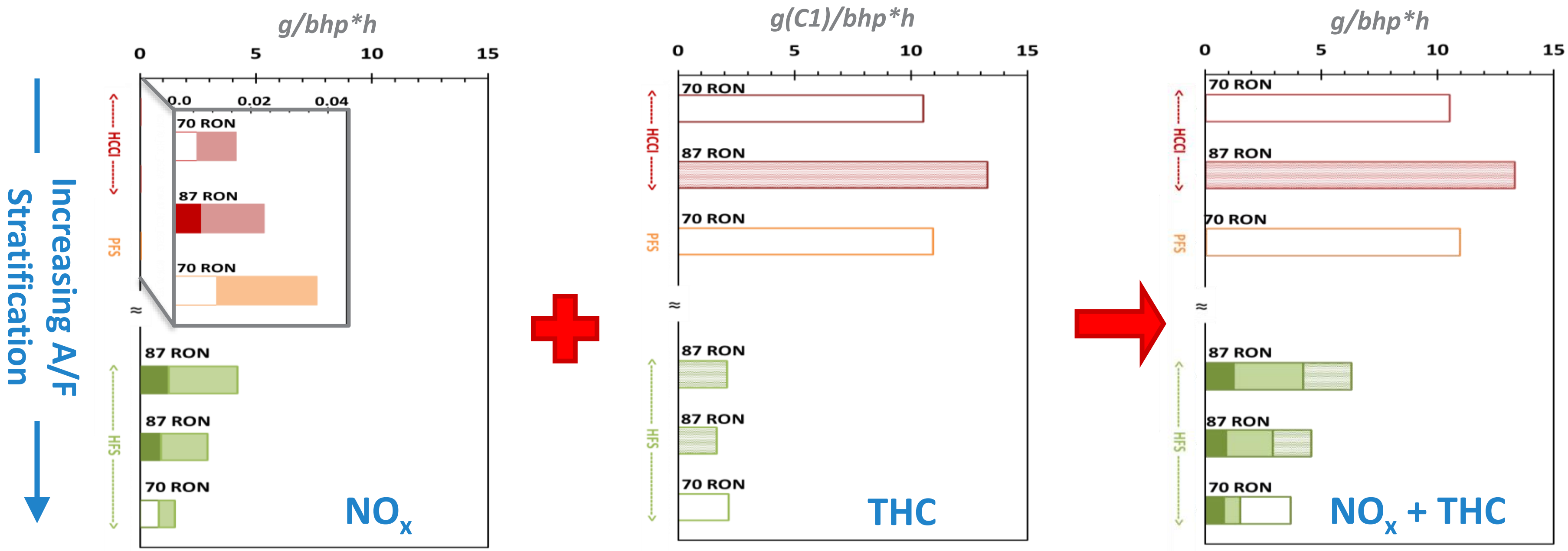
Changes in fuel properties can influence ACI emissions during ACI portion of multimode

Studied 2 gasoline-range fuel

- a low and a high RON
- Similar T40 to T80 distillation curves
- 87 RON has higher aromatic/olefin fraction (15.8% vs. 24.1%)

ACI air-fuel stratification mode has NOx/THC trade-off

Advantages of ACI: High engine efficiency and lower NOx and PM emissions, but NO_x + NMHC combined is now regulated

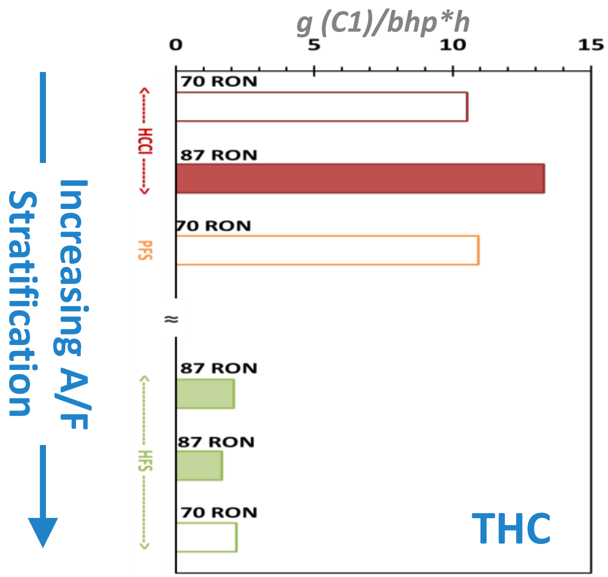


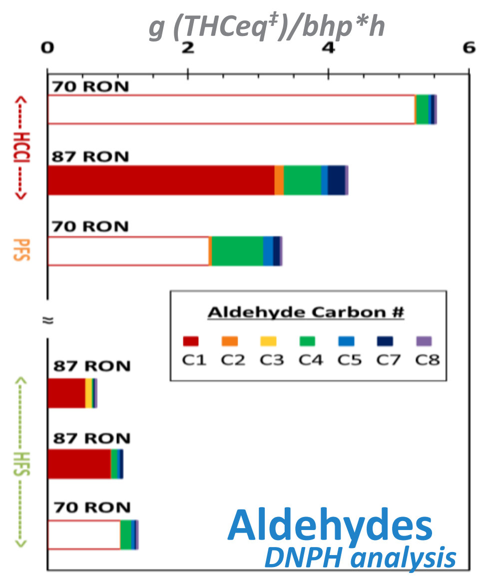
- Air-Fuel Stratification Effect : NOx + THC: 2x ↓ with increasing stratification
  - Less stratification (HCCI & PFS) = NOx: 2 orders of magnitude ↓; THC: more than 2x ↑
    - NOx + THC: 2x ↑, dominated by higher THC
- Fuel Property Effect
  - 87 RON fuel slight ↑ in emissions at same mode (both bookends of stratification)

Fuel Properties & Stratification Mode impact both NOx and THC

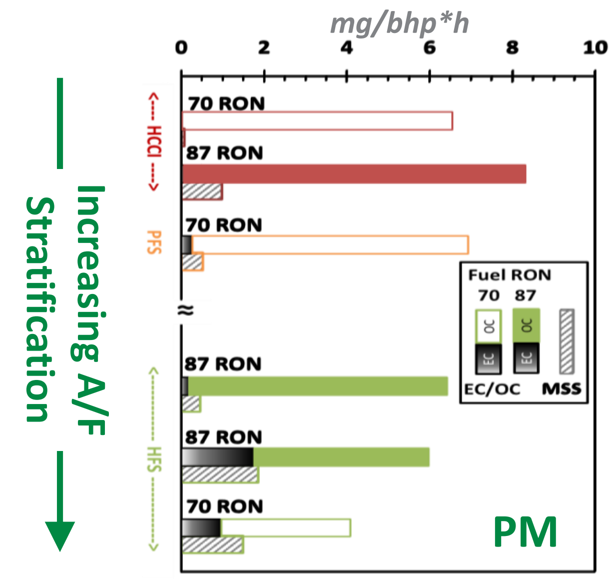
Stratification mode had a NOx / THC trade-off (↓NO_x / ↑ THC)

Complete picture of ACI emissions missing in standard analysis methods





‡CFR40 part 86 (86.144-94)



THC (FID) data does not account for all partial oxidation mass emissions, and accounts for none of the formaldehyde (C1 aldehyde) emissions

- Lower stratification (HCCI & PFS): more than 2x ↑, predominately in formaldehyde
- Accounting for formaldehyde in total THCeq mass ↑ emissions ~20-35%

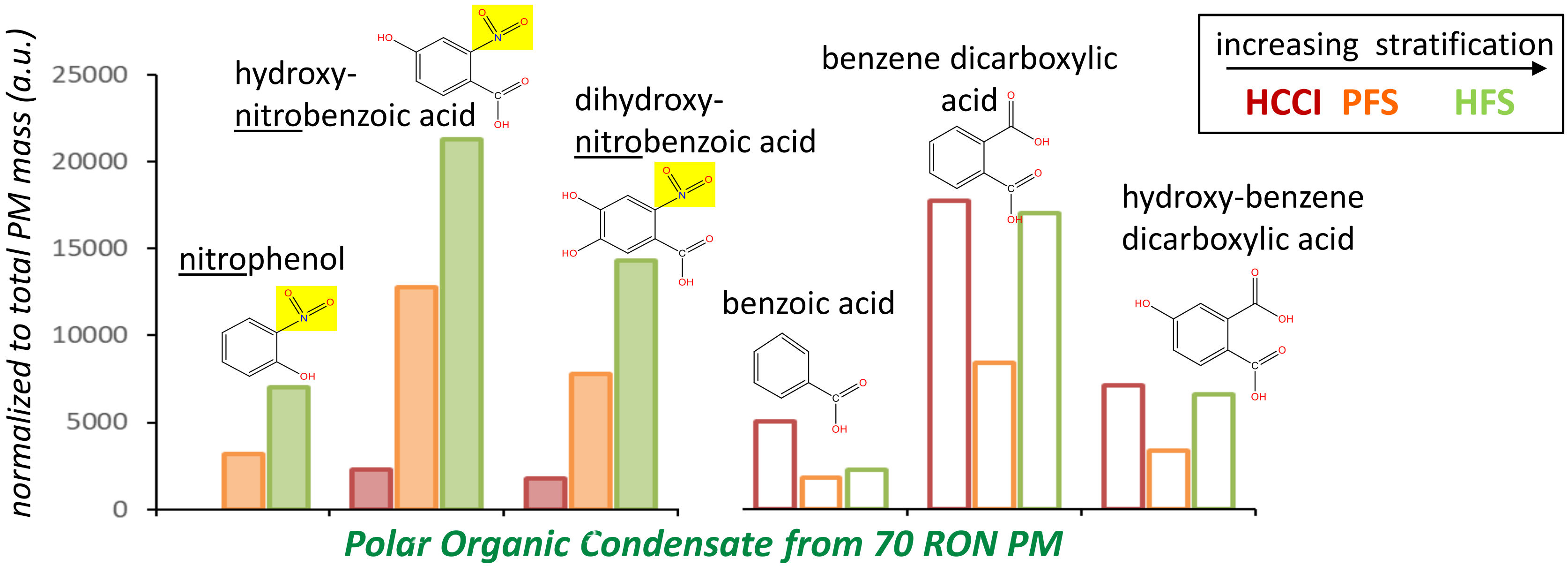
Microsoot Sensor (MSS) data shows low particulate matter (PM) mass, but does not account for organic carbon (OC) in total PM mass

- All stratification modes: ↑ fraction OC in total PM mass, ~100% OC at lower stratification
- RON 87 fuel: slight ↑ in PM mass emissions at same mode comparison

Lower stratification modes increase all types of carbon based mass emissions

Synergistic fuel/stratification combination influences carbon emission chemistry

New analysis method provides insight into partial oxidation process



Chemistry of emissions form partially oxidized carbon can provide insights into incomplete fuel combustion mechanisms

ACI emissions indicated extensive partial oxidation during combustion (lower stratification modes)

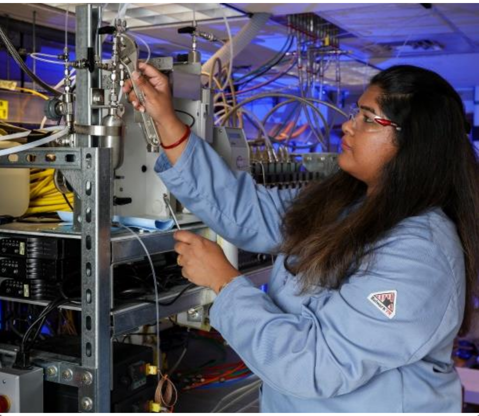
- Gaseous: ↑ THC and ↑ formaldehyde emissions comparable to THC
- PM mass: ↑ Organic Carbon (OC)

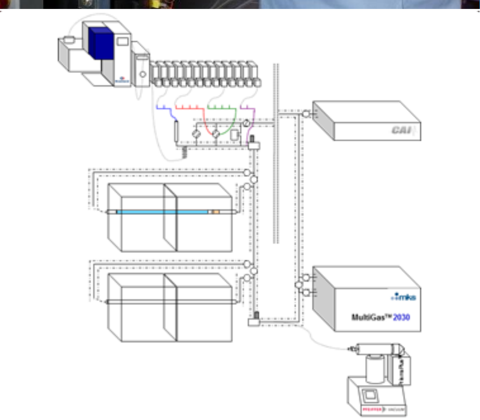
New method developed to study OC PM, specifically polar organic condensates

- Water extraction: targets the nitrogenated and oxygenated organic condensate in PM
- Capillary electrophoresis/mass spectrometry species identification, no fuel/oil interference

Chemistry of incomplete combustion products can feed into ACI predictive modeling efforts on chemical kinetics and emissions formation

E.1.3.1: Fuel Impacts on Emissions Control Performance & Durability





Josh Pihl, Sreshtha Sinha Majumdar, Todd Toops (ORNL)

Relevance:

- Co-Optimized engines + fuels still must meet emissions regulations
- Changes in fuel chemistry may affect catalyst performance, potentially impacting emissions control system compliance, fuel penalty, or cost

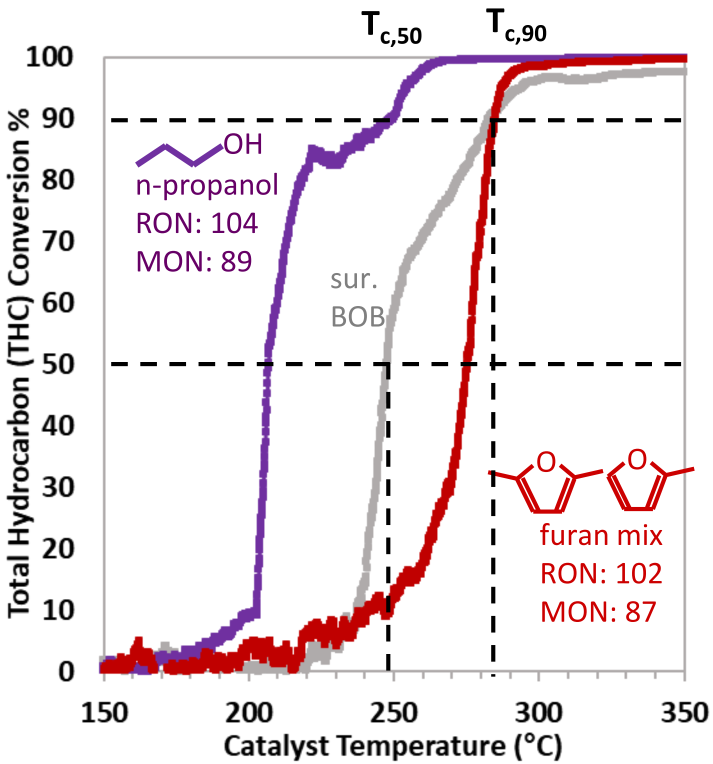
Objectives:

- Identify challenges & opportunities from new fuels
  - catalyst light-off performance during cold start (boosted SI, SI/ACI multimode)
  - catalyst light-down performance during lean operation (SI/ACI multimode)

Approach:

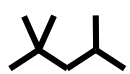
- Use synthetic exhaust flow reactors to measure the impacts of fuel chemistry changes on commercially relevant catalyst materials

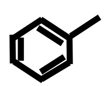
Measured TWC light-off temperatures on a synthetic exhaust flow reactor to capture changes in cold start catalytic activity



synthetic exhaust:	
CO_2	13%
H_2O	13%
CO	0.5%
H_2	0.17%
NO	0.1%
HC (as C_1)	0.3%

surrogate BOB:

65% 

25% 

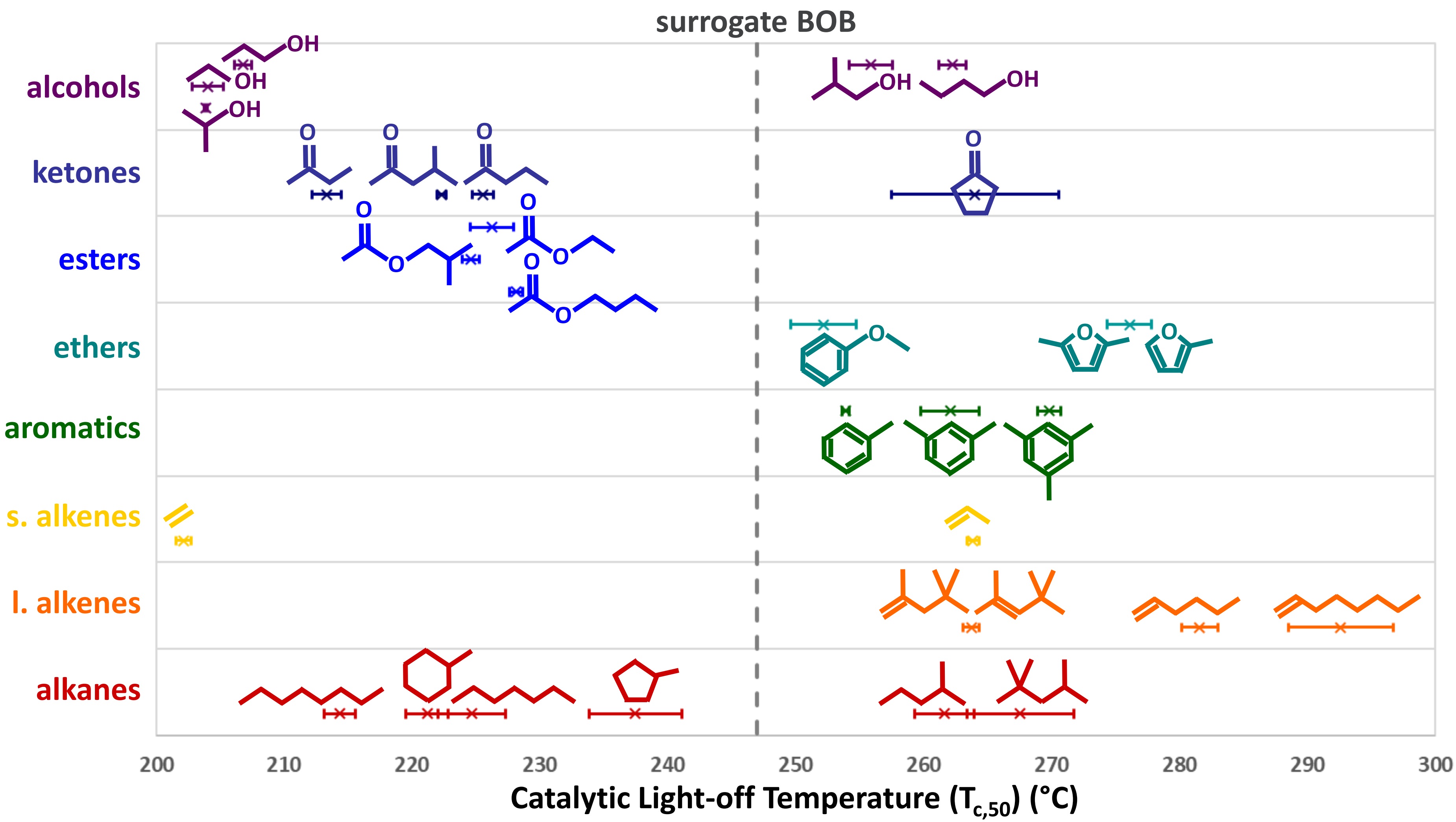
15% 

5% 

- Boosted SI engines rely on TWCs to meet EPA emissions regulations
- Multimode SI/ACI engines will also rely on TWCs at high loads and during cold start
- TWCs do not work when cold, must achieve “light-off” to function
- Changes in fuel chemistry can change TWC light-off behavior
- Synthetic exhaust flow reactor experiments provide a means to measure light-off for a wide range of fuels
  - aged commercial TWC core sample
  - protocols developed by industry*
- TWC light-off does not correlate with gaseous fuel reactivity (RON, MON)

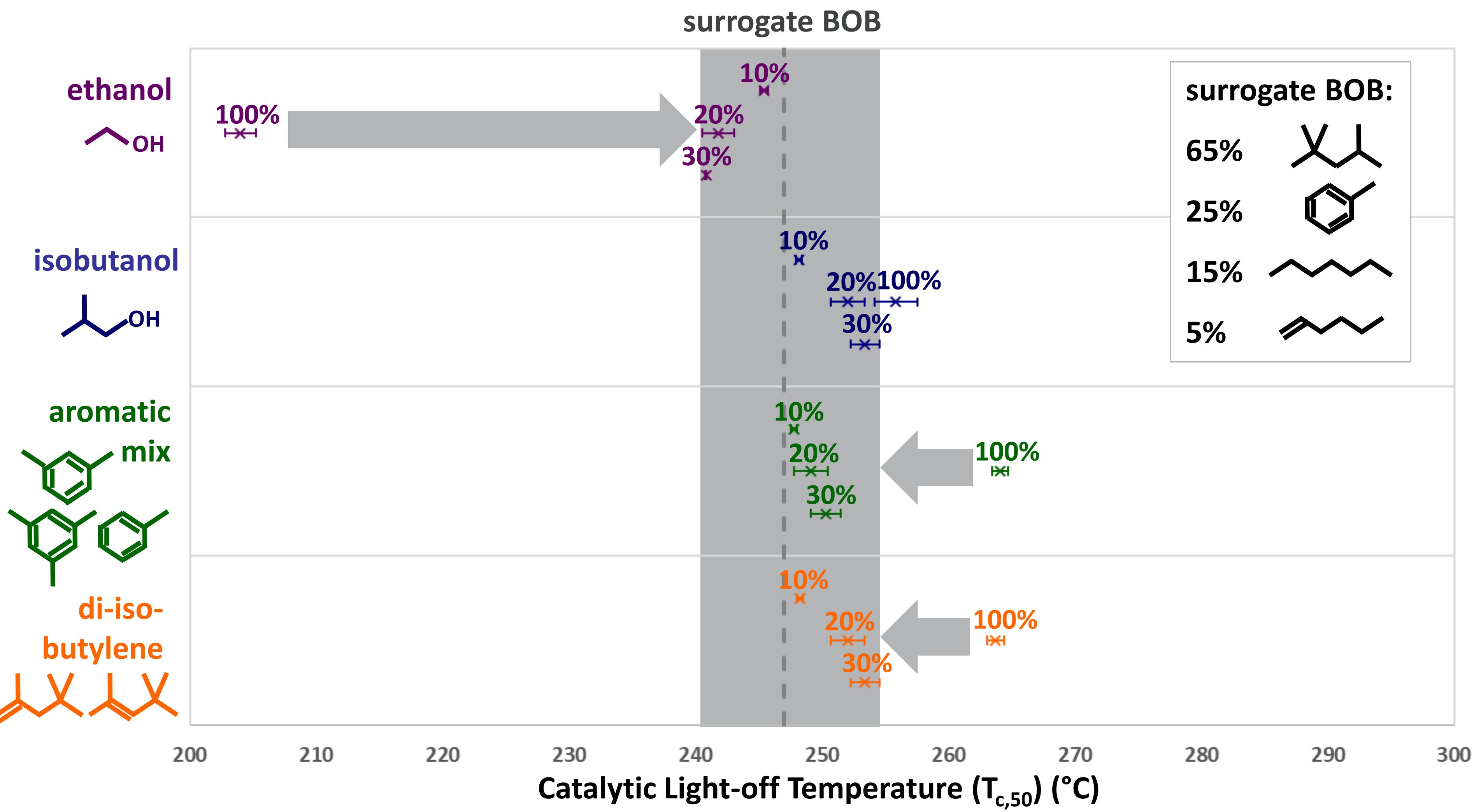
*U.S.DRIVE Low Temperature Oxidation Catalyst Test Protocol

Catalytic reactivity of fuel constituents depends strongly on chemical structure (FY18)



Catalyst light-off performance depends strongly on chemical structure for synthetic exhaust mixtures containing a single organic species

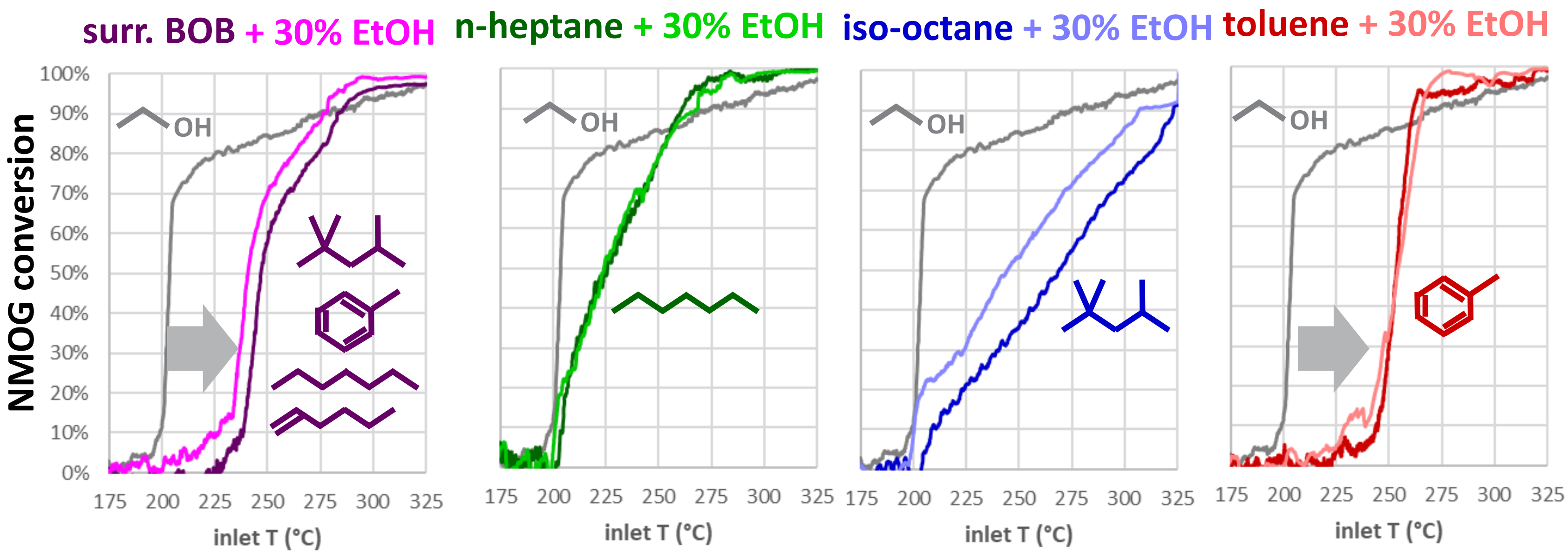
Blends containing 10-30% of various blendstocks in a surrogate BOB all have very similar catalytic light-off behavior



Blends containing up to 30% of Co-Optima blendstocks in a typical BOB will likely neither harm nor help control of gaseous emissions from boosted SI engines

Blend experiments show that aromatic species inhibit catalytic light-off of more reactive fuel constituents

- Conducted dozens of binary & ternary blend experiments to better understand blend light-off behavior



- Observed low T ethanol reactivity over catalyst in mixtures with alkanes
- Observed minimal low T catalytic conversion in mixtures containing toluene
  - Aromatic species are likely blocking catalytic active sites

Taking advantage of fuel constituents with higher catalytic reactivities to improve catalyst light-off will require reducing the aromatic content of the fuel

Collaborative approach:

- Catalyst experiments use protocols developed by the U.S.DRIVE ACEC Tech Team Low Temperature Aftertreatment Working Group
- Catalyst experiments use a surrogate BOB developed by the Co-Optima Fuel Properties team to screen blendstocks
- Fuel blendstock choices are based on Co-Optima High Performance Fuel team recommendations

Dissemination of results:

- Results shared with larger Co-Optima team through presentations to Stakeholder teleconferences and All-Hands meetings
- Emissions and catalysis results are shared with the aftertreatment community though the CLEERS organization, which includes dozens of OEMs and suppliers
- Catalyst light-off results have been presented directly to U.S. OEMs and catalyst suppliers

USDRIVE
DRIVING RESEARCH AND INNOVATION FOR VEHICLE EFFICIENCY AND ENERGY SUSTAINABILITY

Co-Optimization of Fuels & Engines

CLEERS Cross-Cut Lean Exhaust Emissions Reduction Simulations

Remaining Challenges	**Future Work*** *(subject to change with funding levels)*

• Understanding of synergistic effects of fuel properties and ACI combustion modes on emissions
• ACI operation creates new emissions challenges (relative to boosted SI):
  • low exhaust T's
  • high HC emissions
  • lean NOx
  • Increased OC in PM
  • Increased toxic emissions (formaldehyde)
• Potential mitigating or exacerbating effects of fuel chemistry on those challenges is not well understood
	Emissions:
	• Measure detailed gaseous exhaust composition on SI/ACI and full-time ACI engine platforms running with relevant fuels
	  – Fuel boiling range (distillation curve)
	  – Aromatic content
	• Investigate influence of fuel chemistry and engine operating parameters on PM and HC formation in ACI combustion
	Catalysts:
	• Quantify Co-Optima blendstock effects on catalyst light-off and light-down performance (cooling during transition from SI to ACI)
	• Identify potential emissions control architectures for SI/ACI and full-time ACI

**Any proposed future work is subject to change based on funding levels*

Response to FY18 Reviewer Comments

Reviewer Comments	Response
• "..wished that there was convincing information about the active communication among projects."	• Fuel blendstock choices were based on HPF team selection • Surrogate BOB was developed by FP team to screen blendstocks • Presentations on project given at Co-Optima stakeholder and all-hands meetings
• "… a complete evaluation of the project was hard because there was so much crammed into this talk….it is completely unreasonable to cover five projects in a single talk…"	• Co-Optima increased the number of AMR presentations • This AMR presentation included only two projects

Summary

Relevance:

- We need to understand fuel chemical and physical properties, as well as how different modes of ACI operation, impact exhaust composition and performance of emission control devices to predict the effects of multimode combustion and Co-Optima blendstocks on emissions regulations

Approach:

- Utilize unique lab capabilities to develop a fundamental understanding of how changes in fuel chemistry impact emissions and emission control devices

Accomplishments:

- Quantified changes in exhaust composition (PM, NMOG speciation) resulting from the effects of variation in air-fuel stratification of different ACI modes and further contribution caused by a change in fuel properties
- Demonstrated that blends containing up to 30% of Co-Optima blendstocks in a typical BOB will likely neither harm nor help control of gaseous emissions from boosted SI engines, as catalyst light-off is primarily controlled by aromatic content of the BOB

Collaborations:

- CLEERS, ACEC Tech Team, 9 national labs, 20+ universities, 80+ stakeholder organizations

Future Work* (subject to change based on funding levels):

- Evaluate how fuel chemistry composition and physical properties, like aromatic content and distillation curve, change PM and gaseous emissions at different ACI modes with relevant multimode fuels
- Evaluate impact of Co-Optima blendstocks on performance of low T catalyst materials under lean exhaust environments relevant to multimode

**Any proposed future work is subject to change based on funding levels*

PM = particulate matte; NMOG = non-methane; CLEERS = Cross-cut, Lean Exhaust Emissions Reductions Simulations; ACEC= Advanced Combustion & Emissions Control

Technical Back-Up Slides

Multi-Cylinder Engine + PM Setup

- **GM 1.9-L multi-cylinder diesel engine**
  - OEM pistons (CR 16.5)
  - OEM diesel fuel system with DI injectors
  - Variable geometry turbocharger with Cooled high-pressure EGR
- **DRIVVEN control system with Combustion Analysis Toolkit**
  - Full control of DI
  - Cylinder-to-cylinder balancing
- **Aftertreatment integration & emissions characterization**
  - Regulated and unregulated emissions
  - Particulate matter characterization

ORNL Multi-Cylinder 1.9L GM

Number of cylinders	4
Bore [mm]	82.0
Stroke [mm]	90.4
Displacement [L]	1.91
Compression ratio [-]	16.5
IVO [°CA aTDC]	344
IVC [°CA aTDC]	−132
EVO [°CA aTDC]	116
EVC [°CA aTDC]	−340
Rated power [kW]	110
Rated torque [Nm]	315

Acronyms: aTDC = after top dead center; CA = crank angle; EVC = exhaust valve closing; EVO = exhaust valve opening; IVC = intake valve closing; IVO = intake valve opening.